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Hot Molecular Cores and High-Mass Star Formation

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Abstract. This review covers hot cores in the context of high-mass star formation. After giving an overview of chemical processes and diversity during high-mass star formation, it reviews the ‘warm envelope’ phase which probably precedes the formation of hot cores. Some recent determinations of the cosmic-ray ionization rate are discussed, as well as recent evidence for hot cores around low-mass stars. Routes for future hot core research are outlined.

1. Introduction

Named after the Orion Hot Core, hot molecular cores are small ($d \lesssim 0.1$ pc) pockets of warm ($\gtrsim 100$ K) dense ($\gtrsim 10^6$ cm $^{-3}$) molecular gas, which show very rich submillimeter spectra. This definition includes both internally and externally heated clumps near stars of all masses, but the focus of this review is on the case of internal heating by young high-mass stars, which form the majority of known hot cores. This review only outlines basic properties of hot cores with an emphasis on recent developments. Recent reviews on the chemistry of star-forming regions, including hot cores, have been given by van Dishoeck & van der Tak (2000) and Langer et al. (2000); high-mass star formation is discussed by Kurtz et al. (2000), Churchwell (2002) and Garay (this volume).

2. The embedded phase of high-mass star formation

Stars of masses > 8 M $_{\odot}$ spend a significant fraction of their lifetime, $> 10\%$, embedded in their natal molecular clouds. This embedded phase can be subdivided into four observationally different groups of objects: (1) The initial conditions of high-mass star formation should be large mass reservoirs which are local temperature minima and density maxima. Candidate objects in this phase have been found through infrared (Egan et al. 1998; Carey et al. 1998) and submillimeter (Motte et al. 2003) observations. (2) High-mass protostellar objects, where the central star is surrounded by a massive envelope with a centrally peaked temperature distribution (van der Tak et al. 2000a, Sridharan et al. 2002). Close to the star, ices start evaporating off the grains. (3) Hot cores, with large masses of warm and dense molecular gas, and large abundances of complex organic molecules such as CH₃OCH₃ and CH₃OCHO. These species are thought to be the chemical ‘daughter’ products of reactions of evaporated

ice mantle components, their ‘parents’. (4) Small ($d \lesssim 0.1$ pc) pockets of ionized gas, called ultracompact H II regions. The ordering of these phases from ‘cold’ to ‘hot’ may well be an evolutionary sequence, where the ratio of envelope mass to luminosity decreases, although the mass of the original cloud may also play a role. Phases 2 and 3 are accompanied by massive molecular outflows (Beuther et al. 2002), phases 1–3 by CH_3OH masers (Walsh et al. 2001), and H_2O masers can be found in all four phases.

The separation between these four phases is not as clean as in the case of low mass star formation. Massive stars form in groups and the four above phases often occur right next to each other, making it hard to assign a single age to the region. An example is G10.47, where VLA images show peaks in both the NH_3 (4,4) line, which traces warm molecular gas, and in the 1.3 cm continuum, which traces ionized gas (Cesaroni et al. 1998). In W49, Wilner et al. (2001) imaged CH_3CN line and dust continuum emission at 1.4 mm using the BIMA interferometer. The number of hot cores in W49 is about half that of ultracompact H II regions, indicating that the hot core phase lasts \sim half the lifetimes of ultracompact H II regions of $\sim 10^5$ yr. This value agrees well with estimates based on chemical modeling (e.g., Rodgers & Charnley 2001) and with dynamical timescales of molecular outflows. This agreement, together with the lack of spatial ordering of different phases within the region, argues against triggering of star formation by an external event.

3. Chemical processes during high-mass star formation

In the earliest, dense, cold phases prior to star formation, atoms and molecules freeze out onto grain surfaces, which act as catalysts for neutral-neutral reactions. The composition of the resulting grain mantles can be probed by mid-infrared spectroscopy. This technique has developed greatly with the ISO mission and the advent of high-quality spectrographs on 8m-class telescopes. The derived abundances (Table 1) exceed by orders of magnitude the values that can be produced by reactions in the gas phase, with CO as the only exception. The data thus make a strong case for an active grain surface chemistry. Additional evidence comes from the observed isotopic composition (D/H ratio) of evaporated H_2CO and CH_3OH (Charnley et al. 1997).

However, the detailed reaction mechanisms of surface chemistry are not well understood. Laboratory experiments on hydrogenation of CO give conflicting results (Watanabe & Kouchi 2002; Hiraoka et al. 2002), so that the origin of solid CH_3OH is not clear. Also, observational limits on solid HDO are inconsistent with the predictions of surface chemistry models (Dartois et al. 2003).

Considering elemental abundances, it is clear that the observational inventory of the solid state is incomplete. The likely reason is that the major carriers of some elements are undetectable through infrared spectroscopy. For example, the only N-bearing species is NH_3 , which contains only $\approx 5\%$ of elemental nitrogen. The remaining nitrogen could be in the (undetectable) form of N_2 . Similarly, OCS does not make up the full sulphur budget. Submillimeter observations suggest trace amounts ($\lesssim 1\%$) of solid H_2S or SO_2 evaporating, but observations with ISO rule out both species, as well as atomic S, as major sulphur carriers (van der Tak et al. 2003).

Table 1. Composition of grain mantles in star-forming regions

Species	Abundance	Reference
H ₂ O	10 ⁻⁴ of H ₂	Van Dishoeck 1998
NH ₃	≤7% of H ₂ O	Dartois et al. 2002
H ₂ CO	3–6% of H ₂ O	Gibb et al. 2000
CH ₃ OH	3–30% of H ₂ O	Dartois et al. 1999
CO ₂	14–20% of H ₂ O	Gerakines et al. 1999
CO	2–25% of H ₂ O	Tielens et al. 1991
OCS	0.1% of H ₂ O	Palumbo et al. 1997
CH ₄	2–4% of H ₂ O	Boogert et al. 1998
HCOOH	3–7% of H ₂ O	Schutte et al. 1999

After evaporation into the gas phase, the molecules of Table 1 start a complex reaction scheme, building up long carbon chains with many different functional groups. Spectroscopy of hot cores at millimeter wavelengths has revealed considerable chemical complexity: the BIMA survey of CH₃COOH by Remijan et al. (2003) provides a recent example. Probably even larger molecules are formed, but these are very hard to detect, because of spectroscopic confusion, and because individual spectral lines become weaker as the partition function increases for ever larger species.

The formation of large molecules in hot cores is mostly due to NH₃ and CH₃OH, which, after acquiring a proton from H₃⁺, H₃O⁺ or HCO⁺, can form chains. The HCN and C₂H₅OH molecules could play similar roles, but so far, only upper limits on their solid state abundances have been obtained. An important determinant of the chemistry is therefore the competition for protons between NH₃ and CH₃OH, which both have a high proton affinity. Rodgers & Charnley (2001) show model results for various values of the NH₃/CH₃OH ratio, which observations do not yet constrain well.

Chemical diversity can also be the result of high-temperature neutral-neutral reactions. At temperatures $\gtrsim 300$ K, the reactions of O and OH with H₂ drive all the available oxygen into H₂O. Cores at high temperatures are therefore expected to be rich in nitrogen-bearing compounds (Rodgers & Charnley 2001). Although in the models, age differences also cause chemical diversity, observations seem to support a link between temperature and nitrogen-oxygen differentiation. For example, IRAM Plateau de Bure data show that the peak position of nitrogen-bearing species in W3 (OH) has a higher temperature than that of oxygen-bearing species (Wyrowski et al. 1999). Additional support comes from JCMT spectroscopy of the HCN $J = 9 \rightarrow 8$ line at 797 GHz (Boonman et al. 2001). The data show that the HCN abundance in the envelope of the massive young star AFGL 2591 is not constant with radius, but is enhanced by a factor of 100 at small radii where $T \gtrsim 300$ K.

Shocks do not seem as important for the chemistry of high-mass star-forming regions as they are in the low-mass case (e.g., Bachiller et al. 2001).

Still, two molecules suggest that the envelopes of young high-mass stars may have been processed by shocks, although neither one conclusively. First, ISO-SWS data show low ratios of gas-phase to solid-state CO₂ ($\lesssim 0.1$) and the CO₂ gas phase abundance remains low through the 100–300 K temperature regime (Boonman et al. 2003). After evaporating off grains, CO₂ must be promptly destroyed, which shocks can do in reactions with H (Charnley & Kaufman 2000) or perhaps H₂ (Doty et al. 2002; Talbi & Herbst 2002). Second, Hatchell & Viti (2002) measured NS/CS ratios of 0.02–0.05 in a sample of six hot cores and interpreted these as evidence for shocks. The main reactions to form NS require SH and NH which are produced from OH. Shocks use OH to form H₂O and suppress the production of NS. The values of NS/CS=0.001 – 0.01 measured in warm envelopes (van der Tak et al. 2003) may indicate that shocks play a role too. However, for $t = 3 \times 10^4$ yr, the Doty et al. (2002) model of envelope chemistry also predicts NS/CS $\sim 10^{-3}$, so this ratio cannot be used to demonstrate the influence of shocks.

4. Hot cores with cool envelopes

Before the onset of an ultracompact H II region, young high-mass stars are surrounded by envelopes where ice evaporation occurs in the inner parts. Time-dependent chemical models for this phase were constructed by Doty et al. (2002). These models employ standard reaction networks, and the initial conditions resemble those of dark clouds in the outer envelope ($T < 100$ K). In the inner envelope ($T > 100$ K), the initial abundances of the species in Table 1 are enhanced, corresponding to evaporation of ice mantles.

Figure 1 shows results for SO and SO₂ as an example. The evaporation of ice mantles leads to pronounced abundance enhancements ('jumps') for several molecules. Observational evidence for such jumps is mounting: H₂CO, CH₃OH, SO, SO₂ and OCS show jumps at $T \approx 100$ K (van der Tak et al. 2000b; Schöier et al. 2002; van der Tak et al. 2003), likely due to ice evaporation. In contrast, HCN is enhanced at $T \approx 300$ K (Boonman et al. 2001) in the source AFGL 2591. Such an enhancement is a predicted effect of the O \rightarrow H₂O reaction and suggests that in this source, high-temperature gas-phase reactions have started, marking the birth of the hot core phase. However, the abundance jumps have so far been inferred from detailed modeling of single-dish spectra. Millimeter-wave interferometers could resolve the jumps spatially, which would be an important test of current models of envelope chemistry.

A subset of these 'warm envelopes', where the high mid-infrared brightness allows detection of H₃⁺ rovibrational absorption lines, has been used to derive the cosmic-ray ionization rate (van der Tak & van Dishoeck 2000).¹ This process is the main ionization mechanism of dense molecular clouds, regulating for example the influence of magnetic fields on their dynamics. Van der Tak & van Dishoeck compared observations of H₃⁺ absorption and H¹³CO⁺ emission to a small chemical network coupled to detailed models of the sources' structure, to

¹In this paper, the values in the last column of Table 1 were scaled the wrong way around. The conclusions of the paper are not affected though.

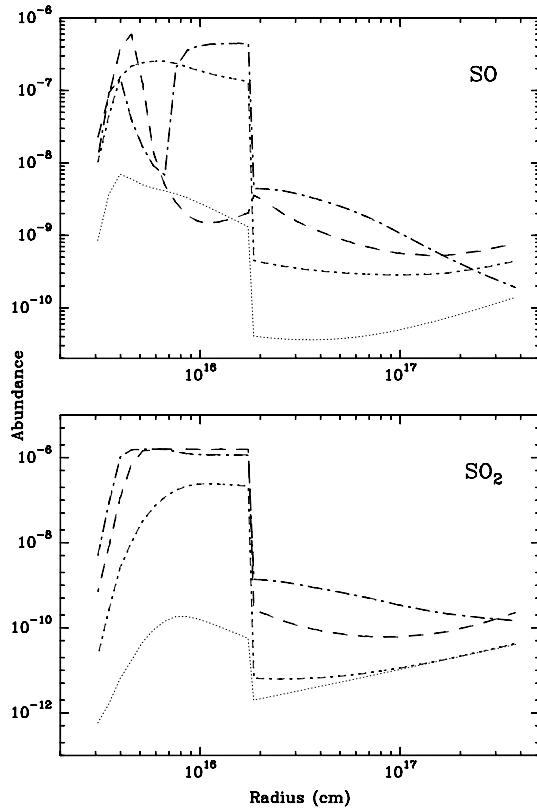


Figure 1. Abundance profiles of gas-phase SO and SO_2 predicted for the envelope of the massive protostar AFGL 2591 for chemical ages of 300, 3000, 30000 and 300000 yr (curves from bottom to top). After Doty et al. 2002.

find a mean ζ of $2.6 \times 10^{-17} \text{ s}^{-1}$. The source-to-source spread of a factor of 2–3 may be correlated with $N(\text{H}_2)$, suggesting that absorption of cosmic rays plays a role. The value of $\zeta = 5.6 \times 10^{-17} \text{ s}^{-1}$ for one particular source was verified by Doty et al. (2002) using a detailed chemical model.²

McCall et al. (2003) infer a much higher value of $\zeta \approx 1 \times 10^{-15} \text{ s}^{-1}$ for the diffuse cloud towards ζ Per. More detailed modeling of the chemistry of H_3^+ and OH and HD, which also depend on ζ , give similar results within a factor of 2–3, $\sim 10 \times$ higher than the results for the massive protostars. McCall et al. propose low-energy cosmic rays that penetrate diffuse but not dense clouds. High-resolution observations of HD in a large sample of diffuse clouds with FUSE will help to test this conclusion.

A much lower value of $\zeta = 0.6 \times 10^{-17} \text{ s}^{-1}$ was obtained by Caselli et al. (2002) for the dense core of L1544. This result needs to be checked in view of the large depletion of CNO-bearing molecules implied by the large abundance of H_2D^+ towards this source (Caselli et al. 2003). If confirmed, this low value of

²In this paper, the predicted $N(\text{H}_3^+)$ should read $5 \times 10^{13} \text{ cm}^{-2}$ rather than $5 \times 10^{14} \text{ cm}^{-2}$.

ζ provides additional evidence for variations in the ionization rates of molecular clouds caused by absorption of cosmic rays. However, more sources need to be studied before local variations in cosmic-ray production can be ruled out.

5. Low-mass hot cores

Although the existence of warm (>100 K) gas in the inner envelopes of low-mass protostars was well-known, it was unclear whether such objects achieved the same chemical complexity as their high-mass counterparts (e.g., Schöier et al. 2002). This situation changed when Cazaux et al. (2003) used the IRAM 30m telescope to detect both 'parent' and 'daughter' type species in the envelope of the low-mass protostar IRAS 16293–2422. The abundances are similar to or perhaps even higher than those in the Orion hot core; the assumed $N(\text{H}_2)$ of the inner envelope of IRAS 16293 and the size of the Orion hot core are critical to this comparison. The high deuterium fractionation of CH_3OH measured by Parise et al. (2002) for IRAS 16293 may also be reproduced by grain surface chemistry models if the atomic D/H ratios from the model of Roberts et al. (2003) are adopted. However, the impact of the rate coefficients of key $\text{H} \leftrightarrow \text{D}$ reactions measured by Gerlich et al. (2002) on the Roberts et al. model needs to be studied.

The initial chemical conditions of low- and high-mass hot cores may well be similar. Using ISAAC on the VLT, Pontoppidan et al. (2003) detected CH_3OH ice in three low-mass young stellar objects. The solid CH_3OH abundances of 15–25% relative to H_2O are comparable to those in the most methanol-rich massive sources. However, it is unclear if evaporation of these ice mantles can drive the rich gas-phase chemistry of IRAS 16293. The measured collapse motions in the envelope imply a travel time for gas through the hot core region of only a few hundred years, which is too short to build up high abundances of complex molecules (Schöier et al. 2002; Rodgers & Charnley 2003).

6. Future directions

Interferometry at (sub)mm wavelengths allows imaging of dust continuum and molecular lines at $1''$ or slightly higher resolution. The contribution by Beuther in this volume shows a recent example obtained with the Sub Millimeter Array. Such data are useful to constrain the temperature and density structure of high-mass star-forming cores, and to determine the multiplicity of their power sources (Wyrowski et al. 1999). However, current instruments can spatially resolve such structure only in a few nearby objects, and searches for kinematic structure in hot cores have just started (e.g., Cesaroni et al. 1998). Efforts are also hampered by limited sensitivity which at the moment prohibits observation of multiple transitions and of isotopic species, which is necessary to determine the optical depth and the excitation of the lines. In the future, ALMA will provide increases in angular resolution and sensitivity by factors of 10 or more.

Observational progress will also come from the HIFI instrument onboard Herschel, which will perform spectral line surveys at heterodyne resolution. Unhindered by the Earth's atmosphere, HIFI will not only probe H_2O (and maybe O_2) directly, but also observe lines that are blocked by atmospheric H_2O (espe-

cially the ground state transitions of hydride molecules). The calibration will be much better than can be achieved from the ground. However, the success of the HIFI mission depends on the availability of spectroscopic and collisional data for astrophysically interesting molecules at frequencies up to 2 THz. Sideband deconvolution is another critical issue (e.g., Comito & Schilke 2002). These caveats are especially important for hot cores with their rich line spectra.

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